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Richard D. James

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University of Minnesota, 200 Oak St. , Minneapolis, MN 55455

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Enclosure 1

DESIGN OF ACTIVE MATERIALS FROM FIRST PRINCIPLES: New transforming materials with unprecedented physical and mechanical properties

Final Report: ARO W911NF-05-1-0261

Richard D. James
University of Minnesota
james@umn.edu

1 Introduction

This is the final report for ARO W911NF-05-1-0261. A detailed progress report was prepared for the Program Manager, Dr. David Stepp in 2006. The final report will be a summary of that one and of work completed from that time to the end of the project. This project has supported the Ph.D. research of Zhiyong Zhang and Krishnan Shankar Narayan.

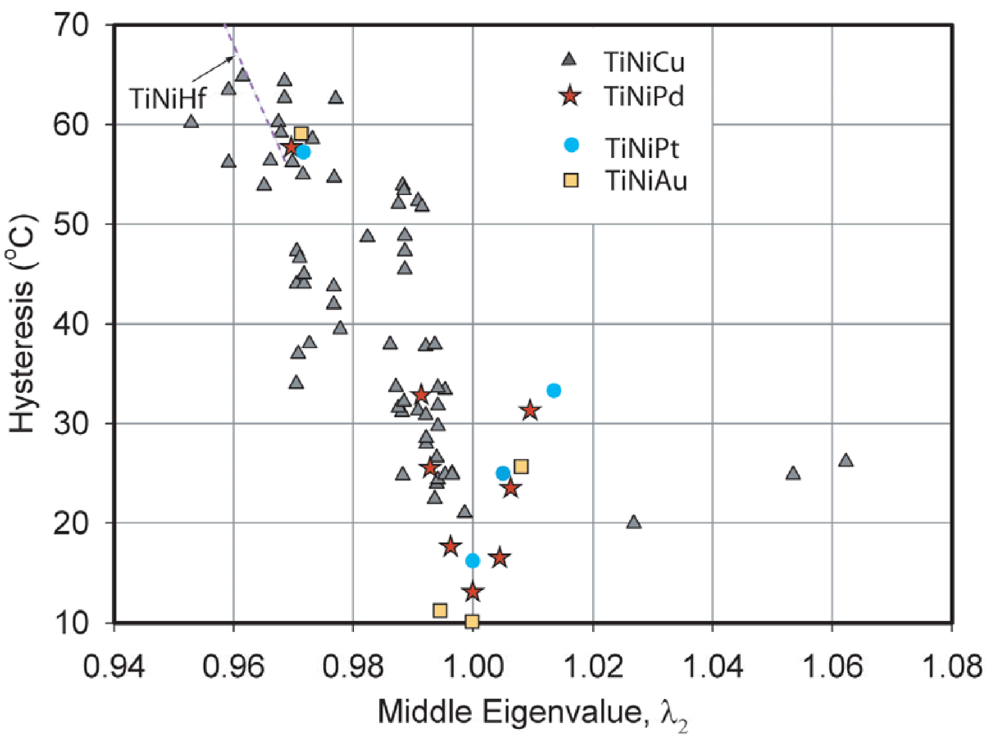

Figure 1: Size of the hysteresis vs. λ_2, the middle eigenvalue of the transformation strain matrix.

2 Main findings

1. A strong correlation has been found between the size of the hysteresis in structural phase transformations and certain special values of the lattice parameters. These special values are associated with conditions of compatibility between the phases. One such condition is seen to have a especially dramatic effect: this is the condition that the middle eigenvalue λ_2 of the transformation strain matrix is 1.

2. We has systematically varied the composition in the system TiNiX, X = Cu, Pd, Pt, Au, to achieve $\lambda_2 = 1$. We found a sharp drop in hysteresis in all cases, see Figure 1.

3. Since hysteresis is a measure of the energy dissipated by the material, there is a strong likelihood that these special conditions also relate to reversibility, i.e., the number of times one can go through the transformation without significant degradation of the material. Literature supporting this has been found (reported in 2006).

4. In recent work [8], we are beginning to understand the relative roles of compatibility and numbers of variants/strains/interfaces. We now have evidence that the latter are also important for behavior, even though they do not have a big effect hysteresis. This is important to understand relative to our condition $\lambda_2 = 1$ vs. our *cofactor conditions.*

5. These discoveries open up the possibility of seeking new families of highly reversible transforming materials. This is especially interesting in cases that the two phases have distinct electromagnetic or optical (EMO) properties. The latter can be expected because EMO properties are generally sensitive to lattice parameters and structural phase transformations have a change of lattice parameters. Promising material systems were identified, with additional information and possible strategies, in the Progress report, 2006. These include highly reversible Cu-based shape memory materials, ferroelectrics near the morphotropic boundary, GMR/CMR materials, fuel-cell compounds ($CsHSO_4$, CsH_2PO_4, $Rb_3H(SeO_4)_2$), multiferroic materials, nonvolatile memory materials in the family $Ge_2Sb_2Te_5$, certain high energy density battery electrode materials, and ferromagnetic shape memory/thermomagnetic alloys. Recently we have noticed that $\lambda_2 = 1$ is nearly satisfied in certain TiTa alloys, an interesting starting point for high transformation temperature highly reversible alloys.

6. These results have attracted very considerable attention worldwide, and several laboratories are now duplicating the results and pushing them in other directions. In particular, programs of tuning lattice parameters for low hysteresis following precisely our conditions on lattice parameters of which we are aware exist at the University of Kiel (E. Quandt), CAESAR Institute in Bonn (Prof. Ludwig), and the University of Bochum (R. Zarnetta, using combinatorial methods), and there is interest also at the State Key Laboratory of Magnetism (Bejing), but I cannot seem to find out details of the latter efforts.

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